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Electron impact double excitation of helium by Glauber approximation

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The $(2s\,2p)^1P$ double excitation cross section of helium by electron impact is investigated in the Glauber method. The standard eight dimensional integral for the amplitude obtained by the Glauber approximation is reduced to a one-dimensional integral which is numerically tractable.

1. Introduction

The phenomenon of double excitation of atomic configurations has been established from the observation of the characteristic emission spectra. Direct photoexcitation from ground state to such excited states is not permissible, but electron impact excitation of them is possible and has been studied theoretically.

For helium atom these quasibound doubly excited states have energies greater than the first ionization threshold. Some of these excited states may, in some cases, couple strongly with the adjacent continuum to emit electron spontaneously and result in the autoionization of the atom. These autoionizing doubly excited states have life-time of the order of the collision time ($\approx 10^{-14}$ sec.).

Doubly excited states of atoms are highly energetic states and they may possess or even exceed the high reactivity of the singly excited ones. Hence they play an important role as initiators of reactions involved in radiation chemistry and in the chemistry of high-temperature gases.

Massey & Mohr (1935) first calculated the cross sections for the excitation by electron impact of the $(2s^2)^1S$, $(2s\,2p)^1P$, $(2s\,3p)^1P$, $(2s\,4p)^1P$ and $(3s\,2p)^1P$ doubly excited states of helium using Born approximation. Becker & Dahler (1964) made a theoretical investigation on some of the doubly excited states of helium, which are stable to autoionization, using Born-Oppenheimer approximation and also the distorted wave and the two-state close coupling approximations. Recently electron impact double excitation cross-sections were calculated by Kullander & Dahler (1972) for several other atoms viz., lithium, beryllium, magnesium and calcium using Born-Oppenheimer approximation.

The cross-sections for electron impact excitation of helium to the doubly excited configurations $(2s\,np)^1P$ and $(ns\,2p)^1P$ (for $n = 2, 3, 4$) have been calculated by Gillespie (1973) in the Born approximation using various Hylleraas type wave functions for the ground state. In the present paper we propose to give a theoretical calculation for the $(2s\,2p)^1P$ excitation of helium by electron impact using the Glauber approximation.

Glauber approximation for scattering amplitudes has recently been applied with considerable success to elastic and inelastic scattering of electrons by helium (Franco 1970, 1973, Yates & Tenny 1972, Thomas & Chan 1973, Chan & Chen 1973, 1974). This approximation has been shown to be more useful than the Born approximation for estimating differential and total cross sections. In view of the excellent agreement of this approximation with the experiment even at the intermediate energy, it seems worthwhile to investigate the problem of double excitation in the same approximation.

2. Theory

The collision amplitude $F_{fi}(\boldsymbol{q})$, when the target helium atom is excited from some initial state i to some final state f by an incident electron is given according to Glauber theory (following the notations and the coordinate systems of Thomas & Gerjuoy 1971) as

$$F_{fi}(\boldsymbol{q}) = \frac{iK_i}{2\pi} \int d\boldsymbol{b} \exp i(\boldsymbol{q}.\boldsymbol{b}) \langle \psi_f(\boldsymbol{r}_2, \boldsymbol{r}_3) | \Gamma(\boldsymbol{b}, \boldsymbol{r}_2, \boldsymbol{r}_3) | \psi_i(\boldsymbol{r}_2, \boldsymbol{r}_3) \rangle, \quad \ldots \quad (1)$$

where

$$\Gamma(\boldsymbol{b}, \boldsymbol{r}_2, \boldsymbol{r}_3) = 1 - \prod_{j=2}^{3} (|\boldsymbol{b} - \boldsymbol{s}_j|/b)^{2i\eta}, \quad \ldots \quad (2)$$

$\boldsymbol{s}_j$ being the projection of $\boldsymbol{r}_j$ on to the plane of $\boldsymbol{b}$ and $\eta = 1/K_i$. Here ψ_i and ψ_f are the wave functions representing the target state before and after collisions. $\boldsymbol{K}_i$ and $\boldsymbol{K}_f$ are respectively the incident and final momenta of the scattering electron and $\boldsymbol{q} = \boldsymbol{K}_i - \boldsymbol{K}_f$ is the momentum transfer, assumed to lie in the plane of $\boldsymbol{b}$. The coordinates of the incident and atomic electrons relative to the nucleus are denoted respectively by $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, $\boldsymbol{r}_3$.

For the doubly excited state of helium, we assume the approximate wave function due to Vinti (1932) as

$$\psi_f(\boldsymbol{r}_2, \boldsymbol{r}_3) = N_{2s, 2p}[\phi_{2s}(Z, r_2)\phi_{2p}(\beta, \boldsymbol{r}_3) + \phi_{2s}(Z, r_3)\phi_{2p}(\beta, \boldsymbol{r}_2)], \quad (3)$$

where $N_{2s, 2p}$ is the normalization factor and ϕ_{2s} and ϕ_{2p} are the corresponding hydrogen like wave functions of a single electron in the field of a charge Z_e and β_e The initial state wave function $(1s^2)^1S$ is similarly given by

$$\psi_i(r_2, r_3) = N_{1s, 1s}[\phi_{1s}(\gamma, r_2)\phi_{1s}(\delta, r_3) + \phi_{1s}(\gamma, r_3)\phi_{1s}(\delta, r_2)]. \quad (4)$$

The values of the parameters are as follows

$$Z = 2.00/a_0, \quad \beta = 1.58/a_0, \quad \gamma = 2.14/a_0 \quad \text{and} \quad \delta = 1.19/a_0.$$

It may be seen easily that in the case of excitation for the magnetic quantum number $m = 0$, $F_{fi}(\boldsymbol{q})$ vanishes. For excitation to either $m = +1$ or -1, the values of $|F_{fi}(\boldsymbol{q})|^2$ are equal. In the present paper, we consider the exicitation for $m = -1$ only. Substituting the initial and final wave functions in eq. (1), we get the expression for scattering amplitude for $(2s\,2p)^1P$ excitation as

$$F_{fi}(\boldsymbol{q}) = 4iK_i\pi N_{2s,\,2p} \times N_{1s,\,1s}[f(a_1, a_2, \boldsymbol{q}) + f(b_1, b_2, \boldsymbol{q})], \quad \ldots \quad (5)$$

where

$$a_1 = \gamma + Z/2, \quad a_2 = \delta + \beta/2, \quad b_1 = \delta + Z/2, \quad b_2 = \gamma + \beta/2$$

and

$$f(x, y, \boldsymbol{q}) = 2\frac{\partial^2 I_0(x, y, \boldsymbol{q})}{\partial x \partial y} + Z\,\frac{\partial^3 I_0(x, y, \boldsymbol{q})}{\partial x^2 \partial y},$$

where the generating function $I_0(x, y, \boldsymbol{q})$ is given by

$$I_0(x, y, \boldsymbol{q}) = \frac{1}{4\pi^2} \int \frac{\exp(-(xr_2 + yr_3))}{r_2 r_3}\, r_3 \sin\theta_3 \exp(-i(\phi - \boldsymbol{q}\cdot\boldsymbol{b}))$$

$$\times \left[1 - \left(\frac{|\boldsymbol{b} - \boldsymbol{s}_2|\,|\boldsymbol{b} - \boldsymbol{s}_3|}{b^2}\right)^{2i\eta}\right] d^2b\, d\boldsymbol{r}_2\, d\boldsymbol{r}_3. \quad \ldots \quad (6)$$

Introducing cylindrical coordinates for $\boldsymbol{r}_2$ and $\boldsymbol{r}_3$, and then using the integral representations for K_0 and J_1 (Abramowitz & Stegun 1964)

$$K_0(x, si) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\exp(-x(Z_i^2 + s_i^2)^{\frac{1}{2}})}{(Z_i^2 + s_i^2)^{\frac{1}{2}}} dZ_i$$

$$\ldots \quad (7)$$

$$J_1(qb) = \frac{1}{2\pi i} \int_0^{2\pi} d\phi_b \exp[i(qb\cos\phi_b \pm \phi_b)],$$

we get

$$I_0(x, y, \boldsymbol{q}) = -8\pi i \int_0^{\infty} b^6 J_1(qb) M_1(xb) M_2(yb) db, \quad \ldots \quad (8)$$

where

$$M_1(u) = \frac{1}{2\pi} \int_0^{\infty} s ds\, K_0(us) \int_0^{2\pi} d\phi (1 + s^2 - 2s\cos\phi)^{i\eta} \quad \ldots \quad (9)$$

and

$$M_2(u) = \frac{1}{2\pi} \int_0^{\infty} s^2 ds\, K_0(us) \int_0^{2\pi} d\phi (1 + s^2 - 2s\cos\phi)^{i\eta} e^{i}$$

Now using the relation (Thomas & Gerjuoy 1971)

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi e^{im\phi}(1+s^2-2s\cos\phi)^{i\eta} = -2^{2i\eta}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\times\int_0^{\infty} dt\, t^{-2i\eta}$$

$$\times\frac{d}{dt}[J_{|m|}(st)\times J_{|m|}(t)], \qquad \ldots (10)$$

and then integrating over s, we get

$$M_1(u) = -2^{2i\eta}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\times\int_0^{\infty} dt\, t^{-2i\eta}\frac{d}{dt}\left[\frac{J_0(t)}{t^2+u^2}\right],$$

$$M_2(u) = -2^{2i\eta}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\times\int_0^{\infty} dt\, t^{-2i\eta}\frac{d}{dt}\left[\frac{2tJ_1(t)}{(t^2+u^2)^2}\right], \qquad \ldots (11)$$

which on further integration gives

$$M_1(u) = u^{-2}[1-(2i\eta)^2(iu)^{-2i\eta}L_{2i\eta-1,\,0}(iu)],$$

$$M_2(u) = 4i\eta u^{-2}[(1+i\eta)(iu)^{-2i\eta-1}L_{2i\eta,1}(iu)-i\eta(iu)^{-2i\eta}L_{2i\eta-1,\,0}(iu)], \qquad \ldots (12)$$

where the modified Lommel function $L_{\lambda,\nu}(iu)$ is defined in terms of the Lommel function $s_{\lambda,\nu}(iu)$ and the modified Bessel function $I_\nu(u)$ as (Thomas & Chan 1973)

$$L_{\lambda,\nu}(iu) \equiv s_{\lambda,\nu}(iu)-ie^{i\pi\lambda/2}2^{\lambda-1}\times\Gamma\left(\frac{\lambda+\nu+1}{2}\right)\Gamma\left(\frac{\lambda-\nu+1}{2}\right)I_\nu(u). \qquad \ldots (13)$$

Hence we get

$$I_0(x, y, q) = \frac{32\eta\pi}{x^2y^2}[(1+i\eta)\int_0^{\infty} b^2db J_1(qb)(iyb)^{-2i\eta-1}\times L_{2i\eta,1}(iyb)$$

$$-i\eta\int_0^{\infty} b^2db J_1(qb)(iyb)^{-2i\eta}\times L_{2i\eta-1,\,0}(iyb)$$

$$+4\eta^2\int_0^{\infty} b^2db J_1(qb)\times\{(1+i\eta)(iyb)^{-2i\eta-1}$$

$$\times L_{2i\eta,1}(iyb)-i\eta(iyb)^{-2i\eta}\times L_{2i\eta-1,\,0}(iyb)\}$$

$$\times(ixb)^{-2i\eta}\times L_{2i\eta-1,\,0}(ixb)]. \qquad \ldots (14)$$

On further integration, we get finally,

$$
\begin{aligned}
I_0(x, y, \boldsymbol{q}) = 32\eta\pi[\Gamma(1+i\eta)\Gamma(2-i\eta)q^{2i\eta-3}\times\{-(1+i\eta)y^{-2i\eta-2}x^{-2}\times \\
\times {}_2F_1(2-i\eta,\, 1-i\eta;\, 2;\, -y^2/q^2) \\
+x^{-2}y^{-2i\eta-2}{}_2F_1(2-i\eta,\, 1-i\eta;\, 1;\, -y^2/q^2)\} \\
+4\eta^2 \int_0^\infty b^6 db\; J_1(qb)\times\{(1+i\eta)(iyb)^{-2i\eta-3}L_{2i\eta,1}(iyb) \\
-i\eta(iyb)^{-2i\eta-2}L_{2i\eta-1,\,0}(iyb)\} \\
\times(ixb)^{-2i\eta-2}L_{2i\eta-1,\,0}(ixb)], \qquad \ldots \quad (15)
\end{aligned}
$$

where Γ and ${}_2F_1$ are the usual gamma and hypergeometric functions respectively.

The expression for the scattering amplitude thus transforms to a single dimensional integral which may be evaluated numerically.

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